
On Spurious Steady-State Solutions of Explicit Runge-Kutta Schemes

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ON SPURIOUS STEADY-STATE SOLUTIONS
OF
EXPLICIT RUNGE-KUTTA SCHEMES

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Abstract

The bifurcation diagram associated with the logistic equation $v^{n+1} = av^n(1 - v^n)$ is by now well known, as is its equivalence to solving the ordinary differential equation (ODE) $u' = \alpha u(1 - u)$ by the explicit Euler difference scheme. It has also been noted by Iserles that other popular difference schemes may not only exhibit period doubling and chaotic phenomena but also possess spurious fixed points. We investigate computationally and analytically Runge-Kutta schemes applied to both the equation $u' = \alpha u(1 - u)$ and the cubic equation $u' = \alpha u(1 - u)(b - u)$, contrasting their behaviour with the explicit Euler scheme. We note their spurious fixed points and periodic orbits. In particular we observe that these may appear below the linearised stability limit of the scheme, and, consequently computation may lead to erroneous results.

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I. Introduction

It is now well established that numerical schemes for solving ordinary differential equations (ODEs) exhibit period-doubling and chaotic behaviour when used with time steps above their linearised stability limit. The most well know example of this is the explicit Euler difference scheme when applied to the ODE

$$u' = \alpha u(1 - u). \quad (1.1)$$

For this equation the scheme becomes

$$u^{n+1} = u^n + \alpha \Delta t u^n (1 - u^n), \quad (1.2)$$

where Δt is the timestep being used. Figure 1 shows the bifurcation diagram obtained for the scheme. The bifurcation diagram is a plot of u^n against $r = \alpha \Delta t$ for two hundred iterates after first 600 iterates have been taken to allow the solution to settle. As can be seen, for $r < 2$, which is the linearised stability limit at the stationary point $u = 1$, all the successive iterates take the value 1, the stable equilibrium of the differential equation. Above this value of r the iterates alternate between two values whilst for even larger values of r the iterates cycle among four distinct values and so on. This phenomenon is known as period doubling, which for this case degenerates to chaotic behaviour where no finite set of distinct values can be discerned. Finally at $r = 3$ the numerical scheme breaks down as its solutions become attracted to the attractor at infinity. Notice however how the period-doubling behaviour is interrupted by solutions of lower periods, a feature of most bifurcation diagrams of simple discrete maps [8]. The numbers labelling the branches of the bifurcation diagram indicate their period (upto period 8), in addition the subscript E on the period one label indicates that it is an essential fixed point – i.e. a fixed point of the ODE (1.1). We shall see later that other, spurious, fixed points may be produced by some numerical schemes.

This type of period doubling behaviour is well known, the above example being equivalent, after a linear transformation, to the logistic equation of population dynamics [6]

$$v^{n+1} = av^n(1 - v^n), \quad (1.3)$$

which is known for its chaotic behaviour.

It is to be noted that once the explicit Euler scheme exceeded its linearised stability limit it announced the fact by its period 2 behaviour where the solution oscillates between two values. This is because linear multistep methods, of which the explicit Euler scheme is a simple example, have only the fixed points of the differential equation (Iserles [2]). This means that if the iterates take on a single value, i.e. a period 1 solution, then this is a solution of the differential equation. However Iserles [2] showed that for the class of Runge-Kutta schemes this need not be the case and, as we shall show later, these schemes can produce spurious solutions which are period 1 (non-oscillatory) but are not solutions to the differential equation. We investigate this phenomenon for three popular Runge-Kutta schemes and observe that such spurious solutions may, in some circumstances, be obtained for values of r below the linearised stability limit. We also note that for these

schemes we must sometimes greatly exceed the linearised stability limit before oscillatory behaviour hints towards a spurious solution which has been present since the limit was reached. Finally we observe that, even for the explicit Euler scheme, more than a single period-doubling solution may exist, the choice being dictated by the initial data, hence bifurcation diagrams become incomplete and fragmented as the iterates jump from one solution to another as r increases. We should note at this point that the explicit Euler scheme can, as well as being a linear multi-step scheme, be considered also as a first order, one-stage Runge-Kutta method.

The implications of behaviour detailed above ranges far beyond pure ODEs. For many steady state calculations for partial differential equations (PDEs) numerical calculations are performed using ODE schemes, often Runge-Kutta, to 'time' march the solution. Could therefore the behaviour observed in this paper explain non-convergence experiences where the solution of the PDE appears to oscillate between more than one steady state, or where the residual will decrease only so far before reaching a plateau? Indeed, even though the mechanisms involved are far more complicated than those studied here, this could well be an explanation. This then leads us to ask if the solutions which are obtained, without any oscillatory behaviour to indicate to the contrary, are the true solutions to the differential equations?

We do not try to answer these questions here, rather initiate studies which one day may allow us to supply such answers with confidence. We not only provide the numerical evidence of bifurcation diagrams, but trace the lower periodic fixed points of the schemes, where possible analytically. A description of the implication of the dynamical behaviour of finite difference methods for practical PDEs in computational fluid dynamics is described in Yee and Yee et al. [10,11]. Reference [11] can also be used as an introductory and state of the art of the current subject. A general account of the theory of asymptotic states of numerical methods applied to initial value problems may be found in Iserles et al. [3].

The schemes considered here are

- 1) Explicit Euler scheme (for comparison)
- 2) Modified Euler (2nd order Runge-Kutta)
- 3) Improved Euler (2nd order Runge-Kutta)
- 4) Heun's scheme (3rd order Runge-Kutta)
- 5) Runge-Kutta 4th order

being tested both on the ODE (1.1) with quadratic forcing term and on the ODE

$$u' = \alpha u(1 - u)(b - u), \quad (1.4)$$

for constant $0 \leq b \leq 1$, with its cubic forcing term.

In the next section we analyse the differential equations and the schemes, finding their fixed points, in Section III we investigate the local behaviour of bifurcations to spurious fixed points, whilst in Section IV we look at the higher order periodic orbits of the numerical schemes.

II. Fixed Points of the Equations and the Schemes

Before we look in depth at the bifurcation diagrams for the schemes applied to the differential equations we first look at some basic theory. We investigate the differential equations themselves, finding their fixed points, before introducing the schemes, finding their fixed points also.

Consider first the general ordinary differential equation

$$u' = f(u), \quad (2.1)$$

where $f(u)$ is a non-linear function of the variable u .

This equation has *fixed points* u^* (also know as *equilibrium points*, *critical points* or *steady-state solutions*) when

$$f(u^*) = 0, \quad (2.2)$$

i.e. when the equation (2.1) is in equilibrium. If the fixed point is *stable* then u will be attracted towards it, otherwise if it is *unstable* then u will be repelled away from it. To discover the stability, or otherwise, of a fixed point u^* we must linearise the differential equation (2.1) about it.

First we set

$$u = u^* + \delta, \quad (2.3)$$

where we refer to δ as a perturbation. Substituting this into the differential equation we obtain

$$\begin{aligned} (u^* + \delta)' &= f(u^* + \delta), \\ &= f(u^*) + \delta f'(u^*) + \dots \end{aligned} \quad (2.4)$$

Since $f(u^*) = 0$ and $u^{*'} = 0$ we have the differential equation for δ

$$\delta' = f'(u^*)\delta + O(\delta^2), \quad (2.5)$$

which, ignoring the $O(\delta^2)$ term, has solution

$$\delta = e^{f'(u^*)t}. \quad (2.6)$$

We now see that if $f'(u^*) > 0$ then the perturbation will grow and so the fixed point is unstable, whereas if $f'(u^*) < 0$ the perturbation will not grow yielding a stable fixed point. If we have $f'(u^*) = 0$ we must consider a higher order perturbation (i.e. not ignore the higher order terms of δ in (2.5)) to determine the nature of the fixed point.

If we turn now to the two differential equations we are considering, namely

$$u' = \alpha u(1 - u) \quad (2.7)$$

and

$$u' = \alpha u(1 - u)(b - u), \quad (2.8)$$

we can find and investigate the stability of their fixed points. For (2.7) we have $f(u) = \alpha u(1 - u)$ which is zero at $u^* = 0$ and $u^* = 1$. The derivative of f is $f'(u) = \alpha(1 - 2u)$ which takes the values $+\alpha$ and $-\alpha$ at these fixed points respectively. Therefore (2.7) has a stable equilibrium point at $u^* = 1$ and an unstable equilibrium point at $u^* = 0$, assuming that α is positive.

For the second ODE (2.8) we have $f(u) = \alpha u(1 - u)(b - u)$ which has zeros at $u^* = 0, 1$ and b . The derivative is

$$f'(u) = \alpha[(1 - u)(b - u) - u(b - u) - u(1 - u)] \quad (2.9)$$

which takes values αb , $\alpha(1 - b)$ and $-\alpha b(1 - b)$ at these fixed points respectively and so, since $0 < b < 1$, we see that $u^* = b$ is a stable equilibrium point whilst $u^* = 0$ and $u^* = 1$ are both unstable.

We next look at the numerical schemes which we are investigating. First there is the *explicit Euler* scheme

$$u^{n+1} = u^n + \Delta t f(u^n), \quad (2.10)$$

which is a linear multistep method. The remainder of the schemes are Runge-Kutta methods, which are non-linear in $f(u)$. The first of these is the second order Runge-Kutta method known as the *modified Euler* scheme and is given by

$$u^{n+1} = u^n + \Delta t f(u^n + \frac{1}{2}\Delta t f(u^n)), \quad (2.11)$$

whilst another second order Runge-Kutta method is the *improved Euler* scheme

$$u^{n+1} = u^n + \frac{1}{2}\Delta t [f(u^n) + f(u^n + \Delta t f(u^n))]. \quad (2.12)$$

The higher order schemes that we investigate are the third order *Heun* scheme

$$\begin{aligned} u^{n+1} &= u^n + \frac{\Delta t}{4}(k_1 + 3k_3), \\ k_1 &= f(u^n), \\ k_2 &= f(u^n + \frac{1}{2}\Delta t k_1), \\ k_3 &= f(u^n + \frac{3}{2}\Delta t k_2), \end{aligned} \quad (2.13)$$

and the *fourth order Runge-Kutta* scheme

$$\begin{aligned} u^{n+1} &= u^n + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4), \\ k_1 &= f(u^n), \\ k_2 &= f(u^n + \frac{1}{2}\Delta t k_1), \\ k_3 &= f(u^n + \frac{1}{2}\Delta t k_2), \\ k_4 &= f(u^n + \Delta t k_3). \end{aligned} \quad (2.14)$$

If we consider a general scheme of the form

$$u^{n+1} = u^n + \Delta t F(u^n, \Delta t), \quad (2.15)$$

which encompasses all those mentioned above for a given $f(u)$, then we can also find the fixed points of the scheme, i.e. u^* such that $F(u^*, \Delta t) = 0$. Here we use the term fixed point to mean a fixed point of period 1 as opposed to a fixed point of higher period (periodic orbit). Note that now these fixed points depend on the additional parameter Δt . We may also investigate the stability of these fixed points in a similar manner to that used to investigate the stability of the fixed points of the differential equation. First we perturb the fixed point, writing $u^n = u^* + \delta^n$, and substitute into (2.15). After expansion of the resulting term on the right-hand side, cancelling of the u^* and neglect of high order terms in δ^n we obtain the difference equation

$$\delta^{n+1} = \delta^n [1 + \Delta t F_u(u^*, \Delta t)] \quad (2.16)$$

for δ^n . This has solution

$$\delta^n = [1 + \Delta t F_u(u^*, \Delta t)]^n \delta^0 \quad (2.17)$$

and so for stability we require

$$|1 + \Delta t F_u(u^*, \Delta t)| < 1, \quad (2.18)$$

i.e.

$$-2 < \Delta t F_u(u^*, \Delta t) < 0. \quad (2.19)$$

Notice again that the parameter Δt appears (maybe not in a linear fashion) and so we shall speak of stability regions for certain ranges of Δt .

Looking at the specific case of the explicit Euler scheme applied to the first ODE (2.7) we have

$$u^{n+1} = u^n + \alpha \Delta t u^n (1 - u^n), \quad (2.20)$$

i.e. $F(u, \Delta t) = f(u) = \alpha u(1 - u)$. This therefore has fixed points $u^* = 0$ and 1, the same as for the differential equation. As noted by Iserles [2] this will always be the case for linear multistep methods. If we now investigate the stability of these fixed points we have $F_u = \alpha(1 - 2u)$ and so (2.19) gives that, for $\Delta t \geq 0$, $u^* = 0$ is unstable, whilst $u^* = 1$ is stable for $0 < \alpha \Delta t < 2$. This is known as the linearised stability range of the scheme applied to the differential equation, and we must choose a Δt within this range if we are to compute the correct stable solution. For the ODEs and schemes we are considering the α may always be combined with the timestep Δt , acting as a scaling, and so for notational brevity we shall from now on use

$$r = \alpha \Delta t. \quad (2.21)$$

The above stability region then becomes $0 < r < 2$.

If we repeat the process with the second ODE (2.8) and the explicit Euler scheme we obtain 0, 1 and b as the fixed points, the first two of which are unstable for $r \geq 0$ whilst the latter (the correct stable equilibrium of the differential equation) is stable for $0 < r < \frac{2}{b(1-b)}$. So, for example in the symmetric case $b = \frac{1}{2}$ we must have $0 < r < 8$.

We may repeat this process for all the combination of schemes and equations, taking welcome aid from an algebraic manipulation package such as MAPLE [5] or DERIVE [1].

The stable fixed points for the various schemes applied to equation (2.7), together with their stability ranges are given in Table 2.1, assuming that $r \geq 0$. The question marks indicate where stable fixed points are known to exist from numerical experiments but no closed analytic form has yet been found.

Scheme	fixed points	stability
Explicit Euler	1	$0 < r < 2$
Modified Euler	1	$0 < r < 2$
	$1 + \frac{2}{r}$	$0 < r < -1 + \sqrt{5} \approx 1.236$
	$\frac{2}{r}$	$2 < r < 1 + \sqrt{5} \approx 3.236$
Improved Euler	1	$0 < r < 2$
	$\frac{2+r \pm \sqrt{r^2-4}}{2r}$	$2 < r < \sqrt{8} \approx 2.828$
Heun	1	$0 < r < 1 + (\sqrt{17} + 4)^{\frac{1}{3}} - (\sqrt{17} + 4)^{-\frac{1}{3}} \approx 2.513$
	?	?
R-K 4	1	$0 < r < \frac{4}{3} + (\frac{172}{27} + \frac{4}{3}\sqrt{29})^{\frac{1}{3}} + (\frac{172}{27} - \frac{4}{3}\sqrt{29})^{\frac{1}{3}} \approx 2.785$
	?	?
	?	?

Table 2.1 Numerical Period 1 Fixed Points of $u' = u(1 - u)$

Scheme	fixed points	stability
Explicit Euler	$\frac{1}{2}$	$0 < r < 8$
Modified Euler	$\frac{1}{2}$	$0 < r < 8$
	$\frac{1 \pm \sqrt{1-8/r}}{2}$	$8 < r < 4(1 + \sqrt{3}) \approx 10.928$
Improved Euler	$\frac{1}{2}$	$0 < r < 8$
	$\frac{1 \pm \sqrt{1-8/r}}{2}$	$8 < r < 12$
	$\frac{1}{2} - \frac{\sqrt{1-12/r}}{4} \pm \frac{\sqrt{1+4/r}}{4}$	$12 < r < 4(1 + \sqrt{6}) \approx 13.798$
	$\frac{1}{2} + \frac{\sqrt{1-12/r}}{4} \pm \frac{\sqrt{1+4/r}}{4}$	$12 < r < 4(1 + \sqrt{6}) \approx 13.798$
Heun	$\frac{1}{2}$	$0 < r < 4(1 + (\sqrt{17} + 4)^{\frac{1}{3}} - (\sqrt{17} + 4)^{-\frac{1}{3}}) \approx 10.051$
	?	?
R-K 4	$\frac{1}{2}$	$0 < r < ?$
	?	?
	?	?

Table 2.2 Numerical Period 1 Fixed Points of $u' = u(1 - u)(\frac{1}{2} - u)$

The stable fixed points for the various schemes applied to equation (2.8) for the special symmetric case $b = \frac{1}{2}$, together with their stability ranges are given in Table 2.2, assuming that $r \geq 0$. The more general case is illustrated by the various Figures (see below). Again question marks indicate where the algebra has defeated us and the algebraic manipulators at our disposal due to the high order polynomials in two variables involved.

Figures 2 – 4 illustrate these fixed points, as well as higher order periodic orbits of the schemes. Again the numeric labelling of the branches denote their period, although some labels for period 4 and 8 are omitted due to the size of the figures. The subscript E on the period one branch indicates the essential fixed point of the differential equation whilst the subscript S indicates the spurious fixed points introduced by the numerical scheme.

The period one orbits in the figures were obtained by solving $F(u^*, \Delta t) = 0$ numerically and checking a discretised version of (2.18), the higher period orbits were obtained by numerical approximations of the conditions of Section III.

As can be seen, except for the explicit Euler scheme (as expected) and the Heun scheme, there are spurious stable fixed points as well as the correct stable fixed point ($u^* = 1$ for (2.7) and $u^* = \frac{1}{2}$ for the symmetric case of (2.8)). Although in the majority of cases these occur for values of r above the linearised stability limit this is not always the case. In particular for the modified Euler scheme applied to (2.7) we see that there is stable spurious orbit below the linearised stability limit of $r = 2$ for $u^* = 1$. This is outside the interval $0 \leq u \leq 1$ and so it is unlikely that it will be picked up accidentally since usually initial value u^0 would be chosen between the two fixed points of the differential equation. The fourth order Runge-Kutta scheme applied to the same equation, however, exhibits a spurious critical path which not only lies below the linearised stability limit but also in the region between the fixed points of the differential equation and so could be easily achieved in practice. For more complicated problems such spurious points could be computed and mistaken for the correct equilibrium.

Another dynamical behaviour of these spurious fixed points generated by the schemes is that when all such spurious paths are plotted for a given combination of equation and scheme they often resemble period doubling bifurcations. On the main branch, where period 1_E lies, the spurious paths are branching from the correct fixed points as they reach the linearised stability limit, and sometimes even forking again as r increases still further. The result of this is that bifurcation diagrams calculated from a single initial condition u^0 will appear to have missing sections of higher period orbits (see Figures 8 – 11), or even seem to jump between branches. This is in fact not the case since all attractors of higher period orbits must be present, although as we shall see such higher period orbits may be non-unique, even for the explicit Euler scheme, thus propagating this effect throughout the bifurcation diagram. In order to compute ‘full’ bifurcation diagrams we must overplot a number of diagrams obtained using different starting values u^0 . For the higher order schemes many such overplots will be needed to fall within all the basins of attraction. Such diagrams are illustrated in Figures 5 – 7, their earlier stages resembling the fixed point diagrams of Figures 2 – 4. The terms *transcritical* and *supercritical* bifurcations [9] refer to the nature of the bifurcation of the fixed point as it reaches its linearised stability limit. Supercritical bifurcations have both of their branches being stable at the bifurcation, whilst for transcritical bifurcations one branch is stable whilst the other (at least initially)

is unstable. As can be seen those solutions with spurious fixed points below the linearised stability limit of the scheme are a result of transcritical bifurcations.

In the next section we make use of perturbation arguments to investigate the local nature of the bifurcations from an essential fixed point of the differential equation to spurious period 1 rest states of explicit Runge-Kutta methods of order ≤ 4 .

III. Bifurcation to Spurious Period One Solutions

In this section we investigate the behaviour of explicit s -stage Runge-Kutta methods of maximum order in the neighbourhood of a stable fixed point u^* of (2.1). It is convenient to express the general s -stage method in the form

$$u^{n+1} = u^n + \Delta t \sum_{j=1}^s c_j f(z_j), \quad (3.1)$$

where

$$z_j = u^n + \Delta t \sum_{l=1}^{j-1} b_{j,l} f(z_l), \quad j = 1, 2, \dots, s \quad (3.2)$$

and, in the more standard notation of the previous section, $k_j = f(z_j)$. In order that we may assume the method to have order s , we shall have to restrict attention to the case $s \leq 4$ [4]. One of the conditions that is necessary for the method to be consistent is that

$$\underline{c}^T \underline{e} = 1 \quad (3.3)$$

where $\underline{c} = (c_1, c_2, \dots, c_s)^T$ and $\underline{e} = (1, 1, \dots, 1)^T$. For a general discussion of bifurcations of maps of the interval we refer to Whitley[9].

Clearly $u^n = u^*$ is a fixed point of (3.1), (3.2) if u^* is such that $f(u^*) = 0$. Expressing the mapping (3.1), (3.2) in the form (2.15) and linearising about u^* we find that

$$\Delta t F_u(u^*, \Delta t) = \rho \underline{c}^T (I - \rho B)^{-1} \underline{e} \quad (3.4)$$

where $\rho = \Delta t f'(u^*)$ and B denotes the $s \times s$ array of weights $b_{j,l}$ that occur in (3.2). With $s \leq 4$, order s may be achieved with s stages and it is a well established result that the Jacobian of the mapping is given by

$$1 + \Delta t F_u(u^*, \Delta t) = 1 + \rho + \frac{1}{2!} \rho^2 + \dots + \frac{1}{s!} \rho^s,$$

an $O(\rho^{s+1})$ approximation to e^ρ . Hence,

$$\underline{c}^T (I - \rho B)^{-1} \underline{e} = 1 + \frac{1}{2!} \rho + \dots + \frac{1}{s!} \rho^{s-1} \quad (3.5)$$

the first s terms in the Taylor expansion of $(e^\rho - 1)/\rho$.

When u^* is a stable fixed point of (2.1) we have $f'(u^*) < 0$ and the linearised stability condition (2.19) will be satisfied for all Δt sufficiently small since, from (3.4) and (3.3)

$$\Delta t F_u(u^*, \Delta t) = \Delta t f'(u^*) + O(\Delta t^2).$$

Hence, u^* will be a stable fixed point of (3.1), (3.2) in some interval $\Delta t \in (0, \Delta t^*]$ or, equivalently, $\rho \in [\rho^*, 0)$ ($\rho^* \equiv \rho^*(s) = \Delta t^* f'(u^*) < 0$). The interval $[\rho^*, 0)$ is usually called the *interval of absolute stability* of the Runge-Kutta method defined by (3.1), (3.2).

It is easily shown that ρ^* satisfies

$$\rho^* \underline{e}^T (I - \rho^* B)^{-1} \underline{e} = -2$$

for $s = 1$ and $s = 3$ so that, by (3.3) and (2.16) $\delta^{n+1} \approx -\delta^n$ as ρ decreases beyond ρ^* leading to a period doubling (flip) bifurcation at $\rho = \rho^*$. This situation will be described briefly in the next section.

In the cases $s = 2$ and $s = 4$ it may be shown that the limit of absolute stability, ρ^* , satisfies

$$\rho^* \underline{e}^T (I - \rho^* B)^{-1} \underline{e} = 0 \quad (3.6)$$

so that $|\delta^{n+1}| > |\delta^n|$ for $\rho < \rho^*$ and there is a loss of stability of the fixed point u^* that would, for a linear problem, lead to $|u^n| \rightarrow \infty$ as $n \rightarrow \infty$. One of our aims here is to show that such divergence does not occur for a genuinely nonlinear differential equation ($f'(u) \neq \text{constant}$) but that there is a bifurcation to a fixed point, \bar{u} , that is spurious in the sense that $f(\bar{u}) \neq 0$ so that it is not a stationary point of (2.1). We also indicate how the nature of the bifurcation is influenced by properties of the method and those of $f(u)$.

Any fixed point, \bar{u} , of (3.1), (3.2) must satisfy

$$\sum_{j=1}^s c_j f(z_j) = 0 \quad (3.7)$$

and

$$z_j = \bar{u} + \Delta t \sum_{l=1}^{j-1} b_{j,l} f(z_l), \quad j = 1, 2, \dots, s. \quad (3.8)$$

Defining

$$\epsilon = \bar{u} - u^*, \quad (3.9)$$

we seek a solution of (3.7) and (3.8) for ρ close to ρ^* (Δt close to Δt^*) in the form

$$\Delta t = \Delta t^* + a\epsilon + b\epsilon^2 + \dots \quad (3.10)$$

and

$$z_j = u^* + \alpha_j \epsilon + \beta_j \epsilon^2 + \gamma_j \epsilon^3 + \dots, \quad j = 1, 2, \dots, s. \quad (3.11)$$

From this we deduce that

$$\begin{aligned} f(z_j) = & \epsilon f'(u^*) \alpha_j + \frac{1}{2} \epsilon^2 [f''(u^*) \alpha_j^2 + 2f'(u^*) \beta_j] \\ & + \epsilon^3 \left[\frac{1}{6} f'''(u^*) \alpha_j^3 + f''(u^*) \alpha_j \beta_j + f'(u^*) \gamma_j \right] + \dots \end{aligned} \quad (3.12)$$

Substituting (3.10)-(3.12) into (3.8) and equating like powers of ϵ leads to

$$(I - \rho^* B) \underline{\alpha} = \underline{e}, \quad (3.13)$$

and

$$(I - \rho^* B)\underline{\beta} = B \left[a f'(u^*)\underline{\alpha} + \frac{1}{2}\Delta t^* f''(u^*)\underline{\alpha}^2 \right] \quad (3.14)$$

where a is to be determined and $\underline{\alpha} = (\alpha_1, \dots, \alpha_n)^T$ and $\underline{\alpha}^2$ denotes the vector whose components are the squares of the corresponding elements of $\underline{\alpha}$. It is convenient for subsequent manipulations to rearrange (3.14) to read

$$\rho^*(I - \rho^* B)\underline{\beta} = [I - (I - \rho^* B)] \left[a f'(u^*)\underline{\alpha} + \frac{1}{2}\Delta t^* f''(u^*)\underline{\alpha}^2 \right]. \quad (3.15)$$

Since (3.6) and (3.13) imply that $\underline{c}^T \underline{\alpha} = 0$ we find, on combining (3.7) and (3.12) and neglecting terms in ϵ^3 , that the condition for a fixed point becomes

$$f''(u^*)\underline{c}^T \underline{\alpha}^2 + 2f'(u^*)\underline{c}^T \underline{\beta} = 0$$

or, with $\rho^* = f'(u^*)\Delta t^*$,

$$\Delta t^* f''(u^*)\underline{c}^T \underline{\alpha}^2 + 2\rho^* \underline{c}^T \underline{\beta} = 0.$$

Taking this together with (3.15) we obtain

$$a = - \frac{\Delta t^* f''(u^*) \underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}^2}{2f'(u^*) \underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}} \quad (3.16)$$

where $\underline{\alpha}$ is given by the solution of the system (3.13). Thus a is well-defined provided that $\underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}$ does not vanish.

When $a \neq 0$, that is, when

$$f''(u^*) \neq 0 \quad (3.17)$$

and

$$\underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}^2 \neq 0 \quad (3.18)$$

there is a transcritical bifurcation given, to first order, by (3.9) and (3.10). The first of these conditions depends on the differential equation (and is violated, for example, for $f(u) = \rho u(1-u)(1/2-u)$ with $u^* = 1/2$) and the second condition depends solely on the Runge-Kutta method.

To study the stability of the bifurcating solution we write

$$\lambda(\epsilon) = 1 + \Delta t F_u(\bar{u}, \Delta t)$$

to denote the Jacobian of the mapping at $\bar{u} = u^* + \epsilon$, $\Delta t = \Delta t^* + a\epsilon + \dots$. We then find that

$$\lambda'(0) = \frac{1}{2}\Delta t^* f''(u^*)\underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}^2$$

and, since $\lambda(0) = 1$, we shall have $\lambda(\epsilon) < 1$ provided

$$\epsilon f''(u^*)\underline{c}^T (I - \rho^* B)^{-1} \underline{\alpha}^2 < 0. \quad (3.19)$$

This condition determines the sign of ϵ that gives rise to a stable branch. Using (3.13), it may be shown that

$$\underline{e}^T(I - \rho^* B)^{-1} \underline{\alpha} = \frac{d}{d\rho}(1 + \rho \underline{e}^T(I - \rho^* B)^{-1} \underline{e})|_{\rho=\rho^*}$$

and, since the argument on the right is a decreasing function of ρ by the definition of interval of absolute stability, it follows that $\underline{e}^T(I - \rho^* B)^{-1} \underline{\alpha} < 0$. This result together with (3.16) imply that the stable branch emanating from $(u^*, \Delta t^*)$ is given by (3.9) and (3.10) for $\alpha \epsilon > 0$, that is $\Delta t > \Delta t^*$.

If we consider the most general second order two stage Runge-Kutta method, it may be parameterised by $\theta (\neq 0)$ so that $\underline{e} = (1 - \theta, \theta)^T$ and

$$B = \begin{pmatrix} 0 & 0 \\ 1/(2\theta) & 0 \end{pmatrix}.$$

It is easily deduced that $\rho^* = -2$, $\underline{e}^T(I - \rho^* B)^{-1} \underline{\alpha} = -1$ for all θ and

$$\underline{e}^T(I - \rho^* B)^{-1} \underline{\alpha}^2 = \frac{1 - 2\theta}{\theta}.$$

Thus, the method will not generate a transcritical bifurcation if $\theta = 1/2$ (the improved Euler method (2.12)). For $\theta \neq 1/2$ we obtain

$$a = \frac{\Delta t^* f''(u^*)}{f'(u^*)} \frac{1 - 2\theta}{\theta}.$$

In particular, for the modified Euler method ($\theta = 1$) with $f(u) = \alpha u(1 - u)$ and $u^* = 1$ we obtain $a = -\Delta t^*$. Thus, from (2.21), (3.9) and (3.10), the bifurcation occurs at $r = 2$ and is described to first order by

$$r \approx 2(2 - \bar{u})$$

and, for stability, $r > 2$ so that $\bar{u} < 1$. These results are seen to agree with the graphical results shown in Figure 2.

For the fourth order Runge-Kutta method, the limit of absolute stability is $\rho^* \approx -2.785$ as given by the negative real root of (3.5) with $s = 4$. Following a tedious calculation we find that (3.16) gives

$$a \approx -0.9598 f''(u^*) / [f'(u^*)]^2$$

so that a transcritical bifurcation always occurs provided $f''(u^*) \neq 0$. The equation of the tangent line at the bifurcation point is given by

$$\bar{u} \approx 1 + 0.521(r - 2.785)$$

for $f(u) = \alpha u(1 - u)$ with $r > 2.785$ so that $\bar{u} > 1$ for stability. These findings agree with the graphical results shown in Figure 2.

In those cases where either (3.17) or (3.18) is not satisfied we find that $a = 0$ in (3.10) and higher order expansions are necessary to determine the nature of the bifurcation. Omitting the details, we determine the coefficient of ϵ^2 in (3.10) to be

$$b = -\frac{\rho^*}{6f'(u^*)^3} \frac{\underline{c}^T(I - \rho^*B)^{-1}\underline{\alpha}^*}{\underline{c}^T(I - \rho^*B)^{-1}\underline{\alpha}} \quad (3.20)$$

where

$$\underline{\alpha}^* = \text{diag}(\underline{\alpha})[(f'(u^*)f'''(u^*) - 3f''(u^*)^2)\underline{\alpha}^2 + 3f''(u^*)^2(I - \rho^*B)^{-1}\underline{\alpha}^2].$$

When $a = 0$ and $b \neq 0$ the bifurcation at $\Delta t = \Delta t^*$ will be of limit point or pitchfork type (see Whitley [9]). Moreover, it will be supercritical if $b > 0$ and subcritical if $b < 0$. Generally speaking the former will be stable and the latter unstable.

Of the examples we have looked at in this section, only the improved Euler scheme leads to a pitchfork bifurcation through violation of condition (3.18). In this case we find that

$$b = \frac{f'(u^*)f'''(u^*) - 3f''(u^*)^2}{3f'(u^*)^3}. \quad (3.21)$$

The other instances of pitchfork bifurcations occur through failure of (3.17) and the expression for b simplifies to

$$b = -\frac{\rho^* f'''(u^*)}{6f'(u^*)^2} \frac{\underline{c}^T(I - \rho^*B)^{-1}\underline{\alpha}^3}{\underline{c}^T(I - \rho^*B)^{-1}\underline{\alpha}}.$$

This leads to

$$b = \frac{f'''(u^*)}{f'(u^*)^2} \frac{1 - 3\theta + 3\theta^2}{3\theta^2} \quad (3.22)$$

for the general second order Runge-Kutta method and

$$b = 2.187 \frac{f'''(u^*)}{f'(u^*)^2}$$

for RK4. The factor involving θ in (3.22) is always positive and it is interesting to note that the value obtained for b is the same for both $\theta = 1$ (modified Euler) and $\theta = \frac{1}{2}$ (improved Euler). This is in accordance with the results shown in Figure 3 (at $\Delta t = 9$, for example). Thus, a (stable) supercritical pitchfork bifurcation results in all cases provided that $f'''(u^*) > 0$. For instance, the function $f(u) = u(1-u)(1/2-u) = -\frac{1}{4}(u - \frac{1}{2}) + (u - \frac{1}{2})^3$ has three real zeros and, with $u^* = \frac{1}{2}$, $f'''(u^*) = 6$. On the other hand, for the function $f(u) = -\frac{1}{4}(u - \frac{1}{2}) - (u - \frac{1}{2})^3$ which has only one real zero, $u^* = \frac{1}{2}$, $f'''(u^*) = -6$ and an (unstable) subcritical pitchfork bifurcation would result.

The perturbation analysis described in this section has shown that it is possible to predict not only the onset of instability at an essential stationary point u^* of the differential system but also to determine the nature of bifurcation that occurs and the stability along the bifurcating branch. In the next section we investigate some of the higher order orbits of

the schemes (a feature not present in the original differential equations which we consider) where consecutive iterates of (2.15) oscillate between two or more values. It was shown earlier in this section that such bifurcations occur for odd order methods. The orbits in these cases are generally much more difficult to obtain analytically, even with the aid of algebraic manipulation software. However, such analysis is presented where possible and numerical backup used for the harder cases.

IV. Periodic Orbits (Fixed Points of Higher Period)

If we use a difference scheme to solve an ODE using a value of r which is slightly above the stability limit for a fixed point of the scheme (either spurious or one belonging to the differential equation) then we often find that the iteration (2.15) will oscillate between two values. This is known as period doubling, a process which is often repeated again at the stability limit for the period two orbit and so on. It is this process which is illustrated by the bifurcation diagrams. As well as period doubling, embedded regions of lower, even odd, periods often occur, frequently as a prelude to chaos. Chaos is the state where there is no finite set of attractors which the iteration visits. Finally instability of the scheme will usually set in when the iterates are attracted to the global attractor at infinity. These latter features are beyond the scope of this paper. We do however investigate the low order periodic orbits of the iteration (2.15) and illustrate that, like the fixed points of the scheme, non-unique stable periodic orbits may co-exist for given values of r . The orbit achieved in these instances will depend on the initial value of the iteration u^0 . In such cases bifurcation diagrams produced using a single u^0 will appear to have parts of their higher order orbits missing, whereas the true situation is the selection of only one of the possible lower period orbits. Bifurcation diagrams therefore can be data dependant, the full diagram only being obtained by the super-position of several such 'sub' diagrams.

Consider the case of period two orbits. This means that there must exist two values u° and u^* such that

$$\begin{aligned} u^\circ &= u^* + \Delta t F(u^*, \Delta t) \\ u^* &= u^\circ + \Delta t F(u^\circ, \Delta t), \end{aligned} \quad (4.1)$$

that is,

$$F(u^\circ, \Delta t) + F(u^*, \Delta t) = 0. \quad (4.2)$$

Rewriting this in terms of just one of the values, u^* say, we have that period two orbit states are given by the solutions of the equation

$$F(u^*, \Delta t) + F(u^* + \Delta t F(u^*, \Delta t), \Delta t) = 0. \quad (4.3)$$

There are likely to be more than two solutions of (4.3) and so they must be paired using (4.2). Note that the fixed points of the scheme will also satisfy both (4.2) and (4.3).

To investigate the stability of the period two orbits we again perturb them slightly. For schemes of the form (2.15) which we are considering this amounts to the following (see e.g. Sleeman et al [7] for a technique applied to linear multistep schemes). Perturb the orbit state to $u^{n-1} = u^* + \delta^{n-1}$ then linearising

$$u^{n+1} = u^{n-1} + \Delta t [F(u^{n-1}, \Delta t) + F(u^{n-1} + \Delta t F(u^{n-1}, \Delta t), \Delta t)] \quad (4.4)$$

about u^* gives

$$\delta^{n+1} = \delta^{n-1} [1 + \Delta t F_u(u^*, \Delta t)] [1 + \Delta t F_u(u^* + \Delta t F(u^*, \Delta t), \Delta t)] \quad (4.5)$$

and so we see that for stability of the orbit we require

$$|[1 + \Delta t F_u(u^*, \Delta t)] [1 + \Delta t F_u(u^* + \Delta t F(u^*, \Delta t), \Delta t)]| < 1. \quad (4.6)$$

These calculations are too involved for the higher order schemes that we are considering, however we present the analytic forms for the period two orbits of the explicit Euler scheme in Table 4.1.

Equation	period 2 orbits	stability
$u' = \alpha u(1 - u)$	$\frac{r+2 \pm \sqrt{r^2-4}}{2r}$	$2 < r < \sqrt{6} \approx 2.4495$
$u' = \alpha u(1 - u)(\frac{1}{2} - u)$	$\frac{1 \pm \sqrt{1-8/r}}{2}$	$8 < r < 12$
	$\frac{1}{2} - \frac{\sqrt{1-12/r}}{4} \pm \frac{\sqrt{1+4/r}}{4}$	$12 < r < 14$
	$\frac{1}{2} + \frac{\sqrt{1-12/r}}{4} \pm \frac{\sqrt{1+4/r}}{4}$	$12 < r < 14$

Table 4.1 Period 2 Orbits of the Explicit Euler Scheme

We note two things. Firstly that the period two orbits for the explicit Euler scheme are exactly the spurious fixed points of the improved Euler method, although their stability range is different. This is not too surprising when one considers that (4.3) with $F(u, \Delta t) \equiv f(u)$, as is the case for the explicit Euler scheme, is precisely the equation for the fixed points of the improved Euler scheme. Secondly we note that for the second equation, (2.8), there are three different period two orbits, two of which co-exist over a range of r . We remark on this to point out that although linear multistep schemes possess only the fixed points of the equations their higher period orbits can be non-unique.

Although we do not present analytic forms for the orbits (except those above), the orbits, upto period 8, depicted in Figures 2 – 4 were obtained by numerically solving (4.3), or the appropriate higher order form, and checking a discretised form of the appropriate stability condition, for example (4.6).

Finally complete bifurcation diagrams for the various combinations of schemes and equations, including cases of (2.8) where $b \neq \frac{1}{2}$, are shown in Figures 5 – 7, whilst bifurcation diagrams produced using only a single initial data u^0 are given in Figures 8 – 11 illustrating the apparent missing of branches described above, together with the corresponding full bifurcation diagrams obtained by overlaying multiple single data diagrams.

V. Summary

We have investigated the fixed points and periodic orbits of four Runge-Kutta schemes, contrasting them with those of the explicit Euler scheme which is known to possess only the fixed points of the differential equation. We have seen how not only do these schemes produce spurious fixed points but that these spurious features of the schemes can manifest themselves below the linearised stability limit for the correct fixed points. This raises the possibility of erroneous results when such schemes are used for computations on problems where the correct result is not known *a priori*. We have also observed how multiple orbits of a given period may co-exist, the particular one selected by the scheme depending on the initial data. Thus bifurcation diagrams produced using a single starting value may appear to be missing branches of higher order orbits.

Future work will be directed towards investigation into the effect of using such ODE solvers for the source term component of reaction-convection equations.

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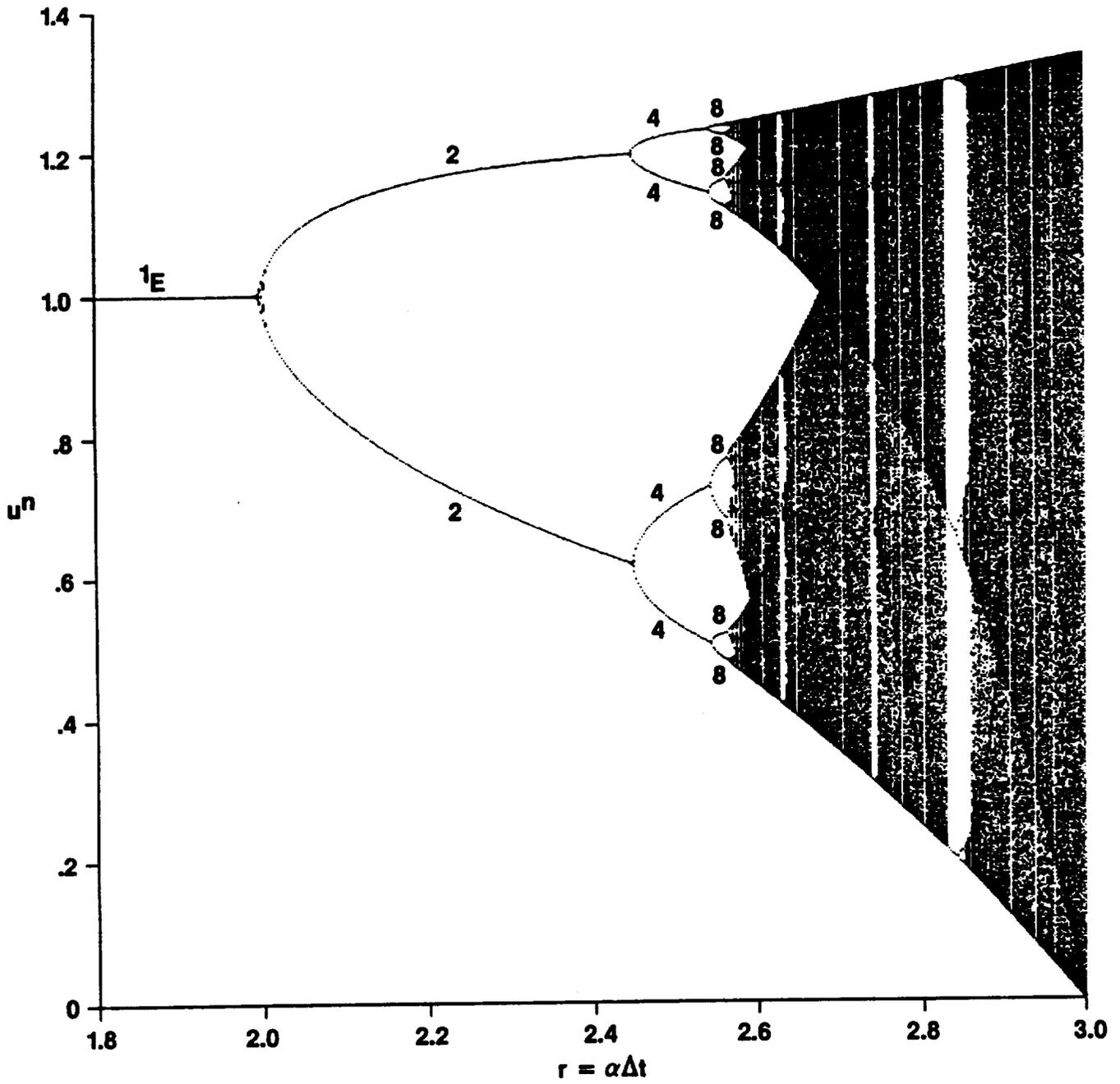


Figure 1. Bifurcation diagram for the Euler scheme applied to $u' = \alpha u(1 - u)$.

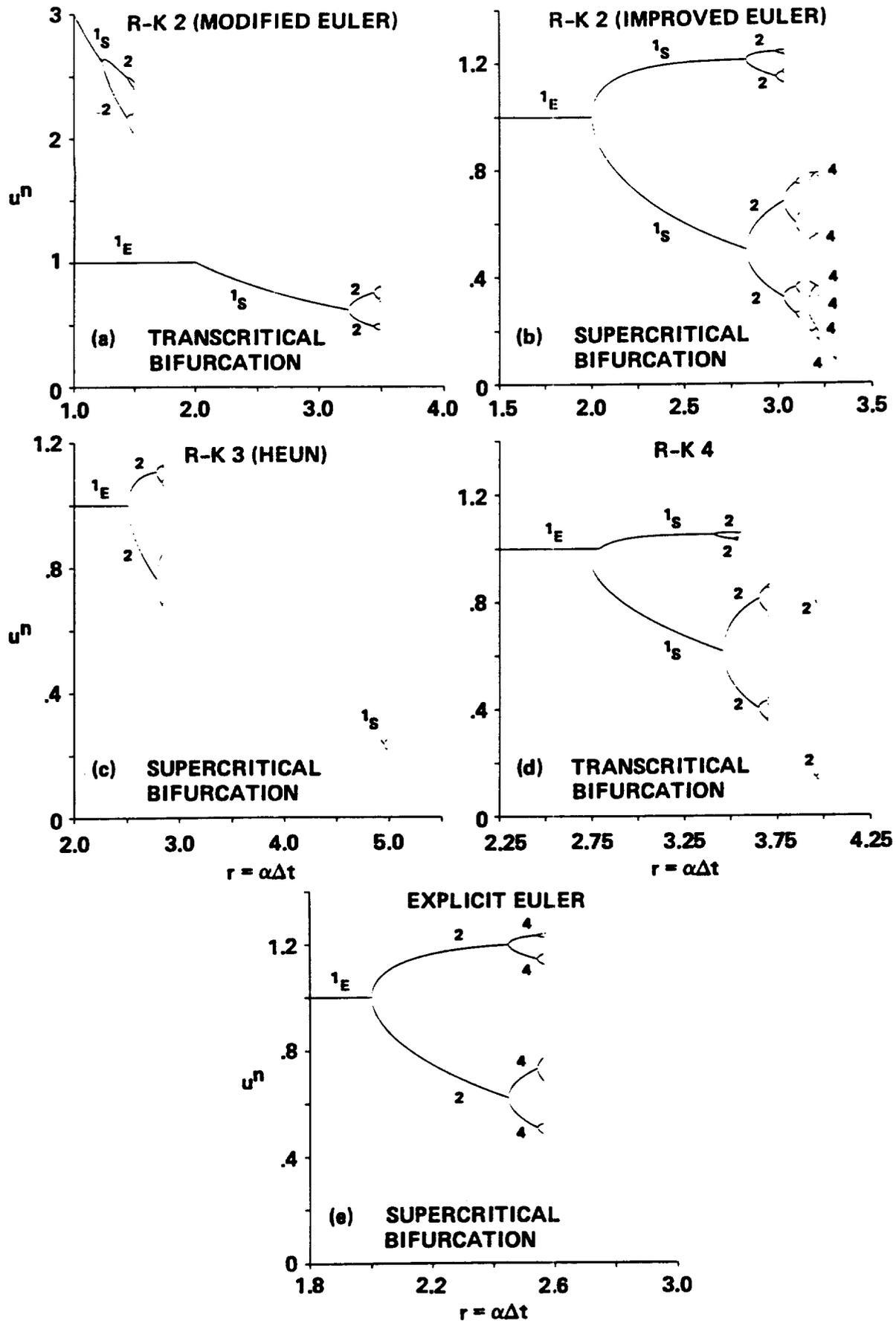


Figure 2. Stable fixed points of period 1,2,4,8 for $u' = \alpha u(1 - u)$.

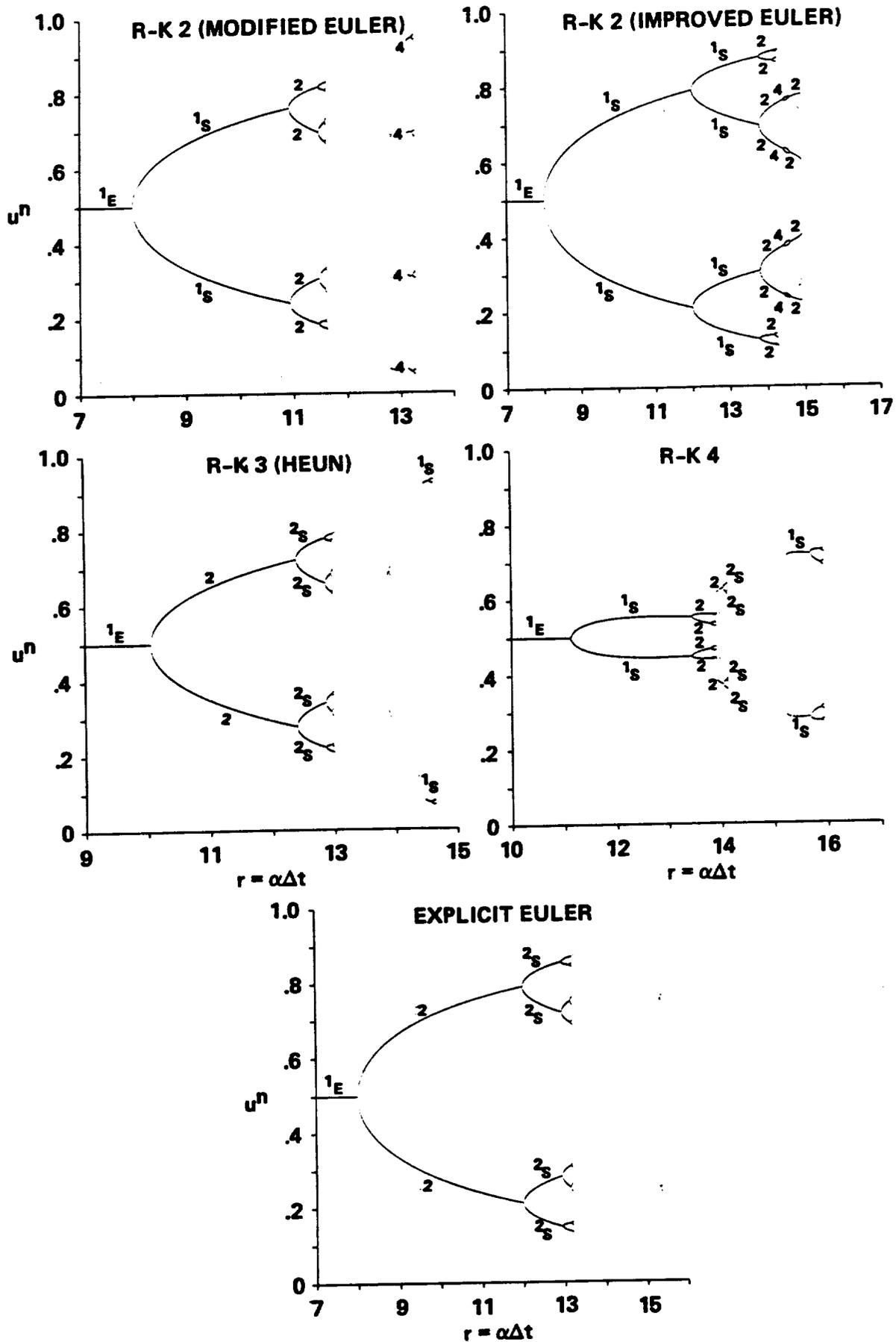


Figure 3. Stable fixed points of period 1,2,4,8 for $u' = \alpha u(1 - u)(1/2 - u)$.

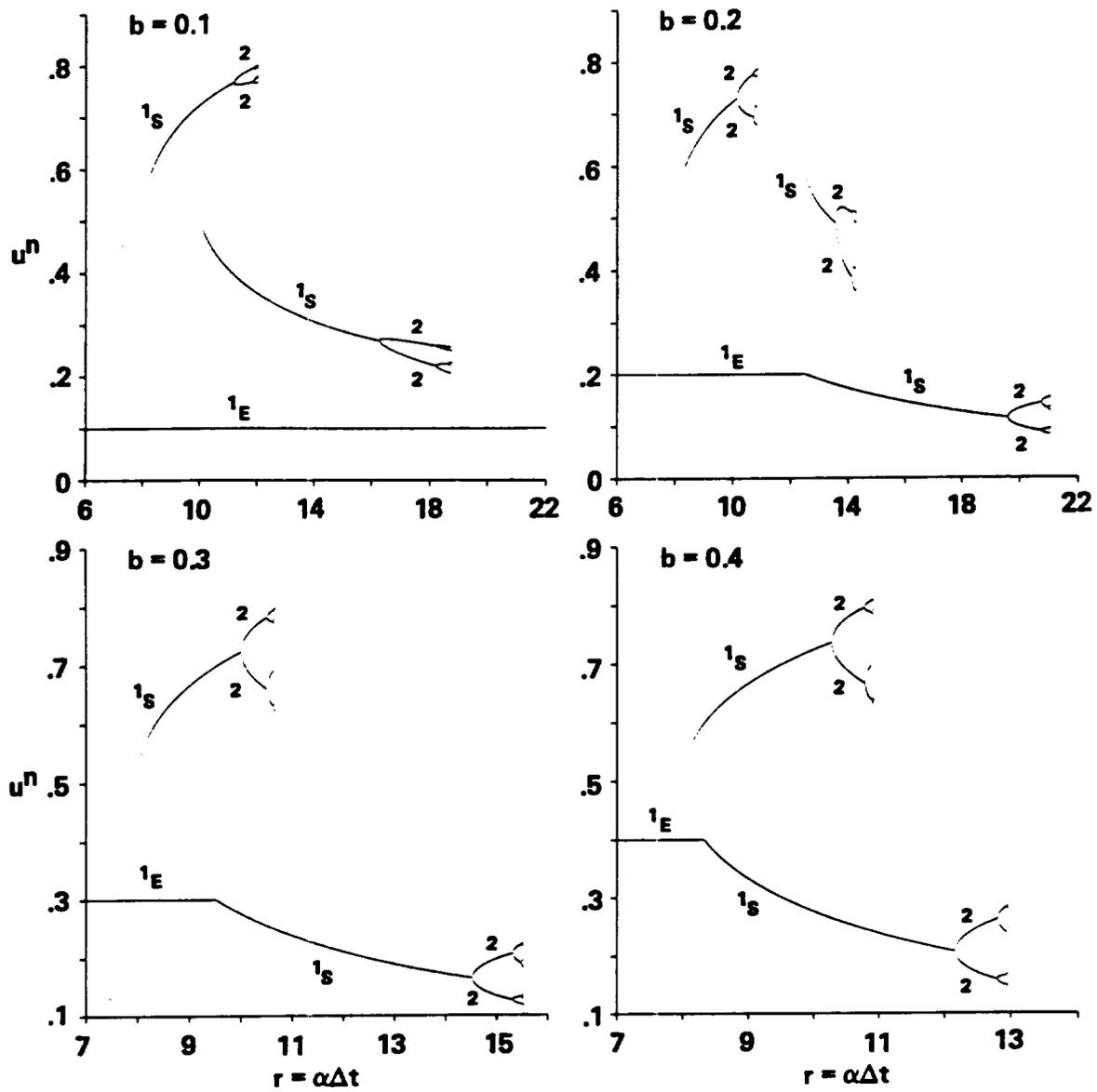


Figure 4. Stable fixed points of period 1,2,4,8 for Modified Euler (R-K 2) scheme applied to $u' = \alpha u(1-u)(b-u)$.

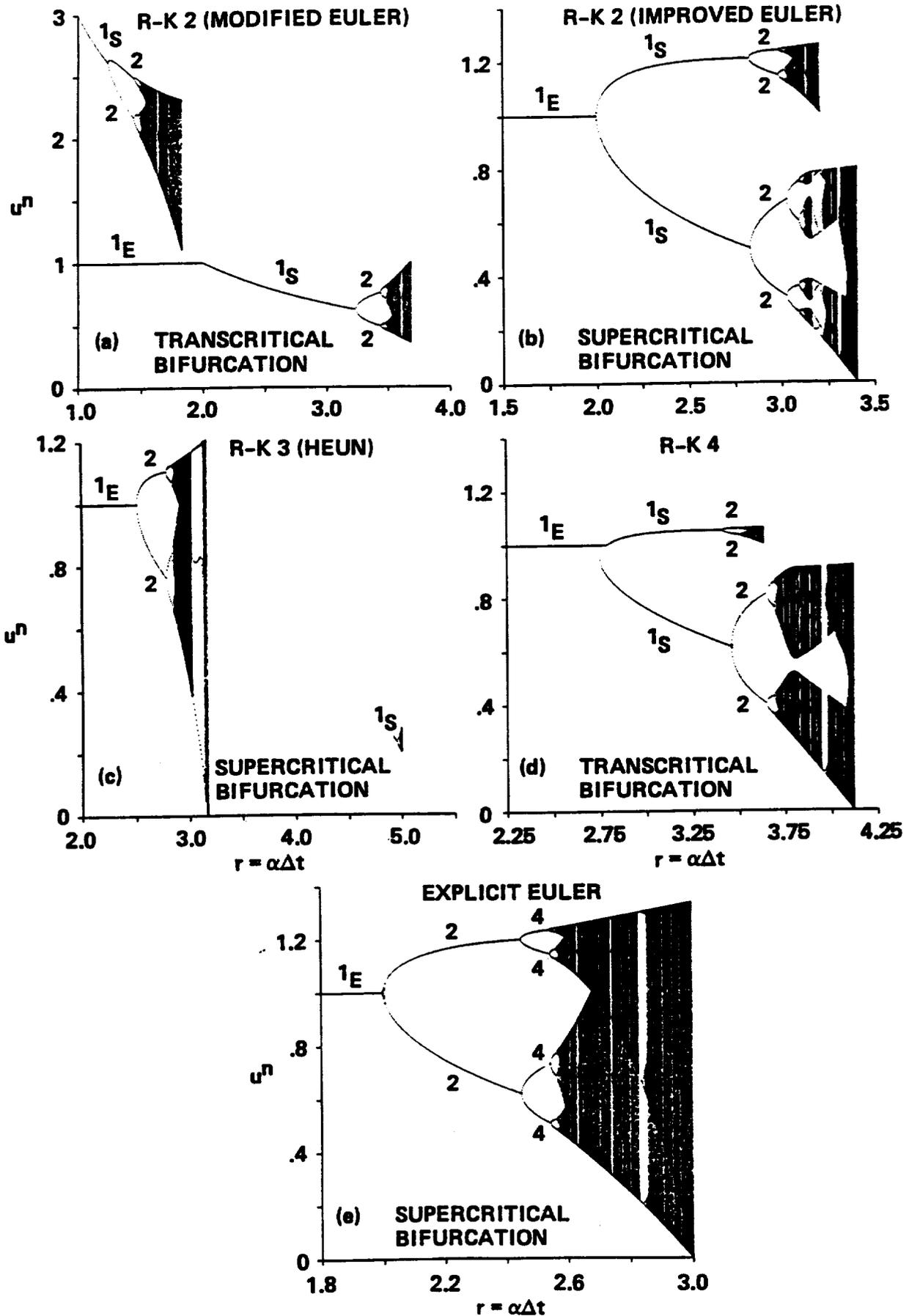


Figure 5. Bifurcation diagrams for $u' = \alpha u(1 - u)$.

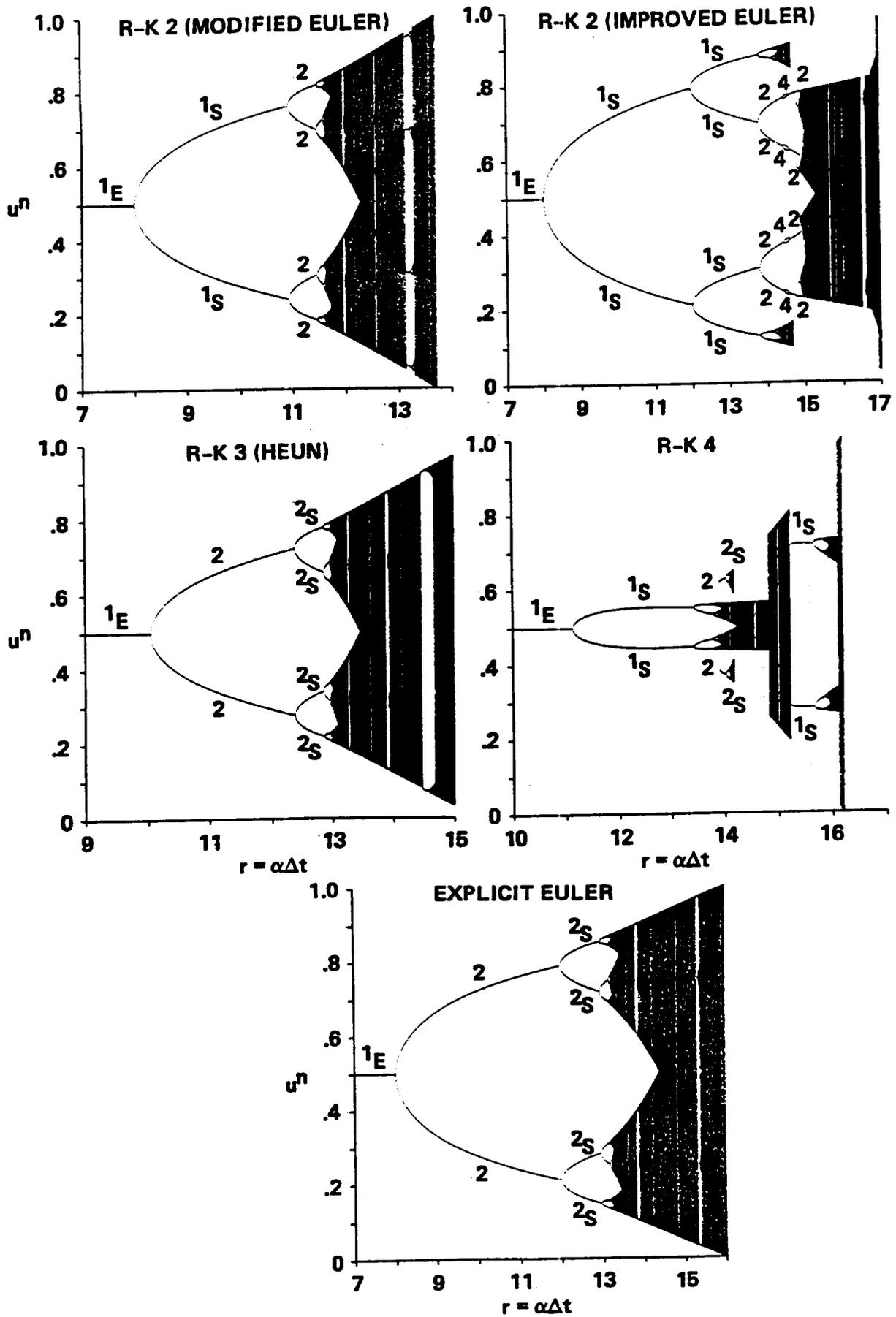


Figure 6. Bifurcation diagrams (supercritical) for $u' = \alpha u(1-u)(1/2-u)$.

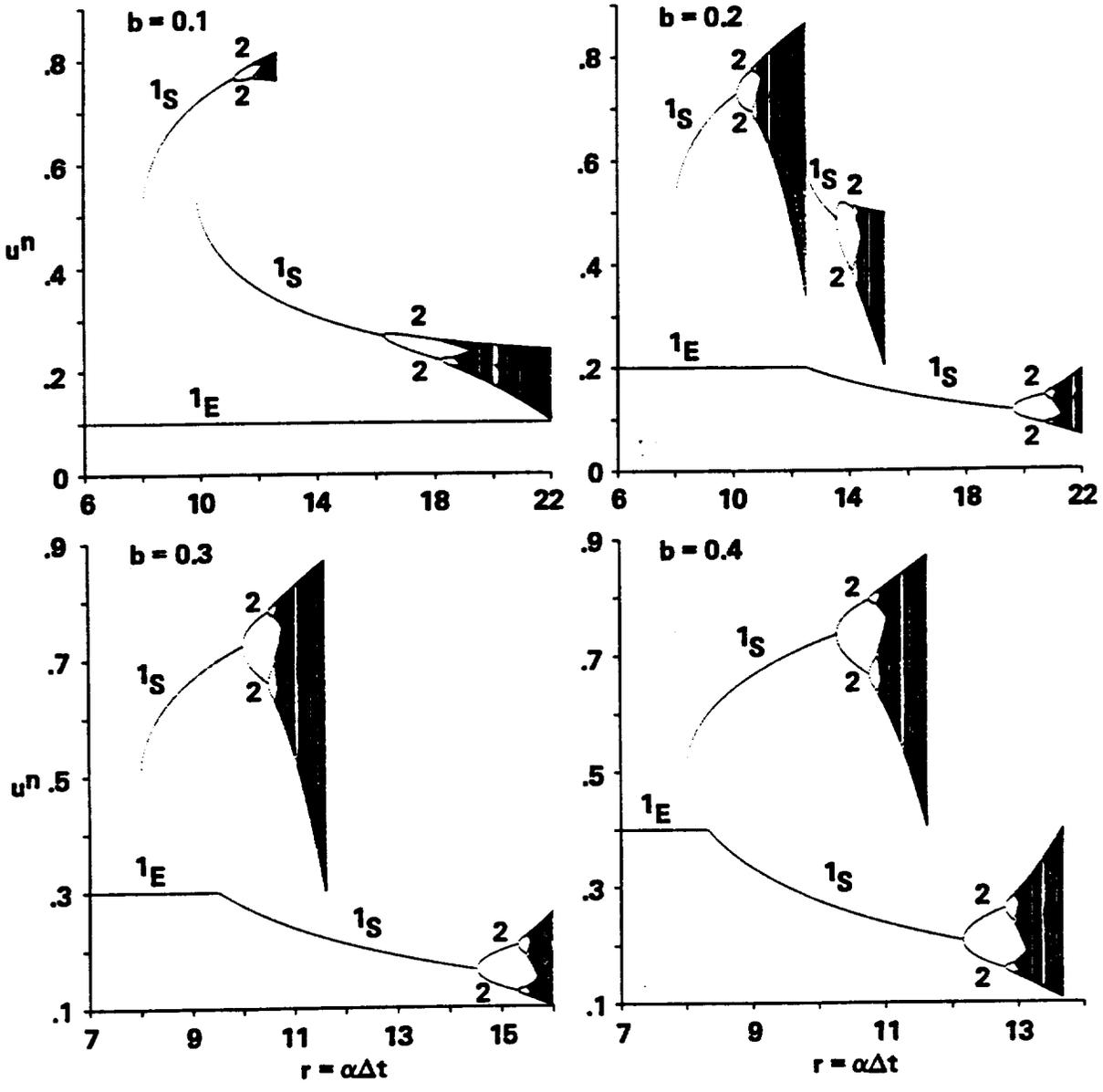


Figure 7. Bifurcation diagrams (transcritical) for Modified Euler (R-K 2) scheme applied to $u' = \alpha u(1-u)(b-u)$.

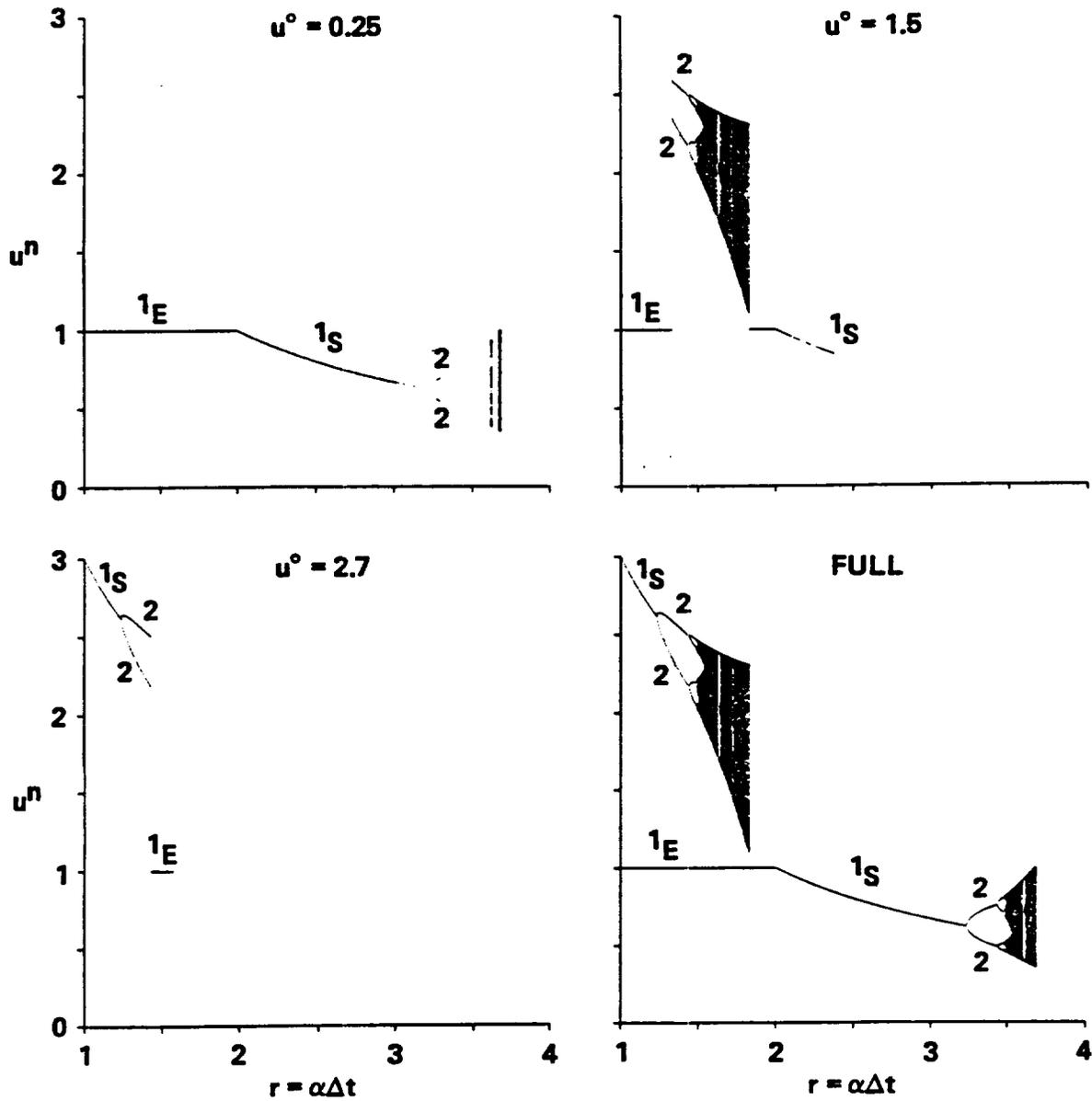


Figure 8. Bifurcation diagrams (transcritical) for Modified Euler (R-K 2) scheme applied to $u' = \alpha u(1 - u)$.

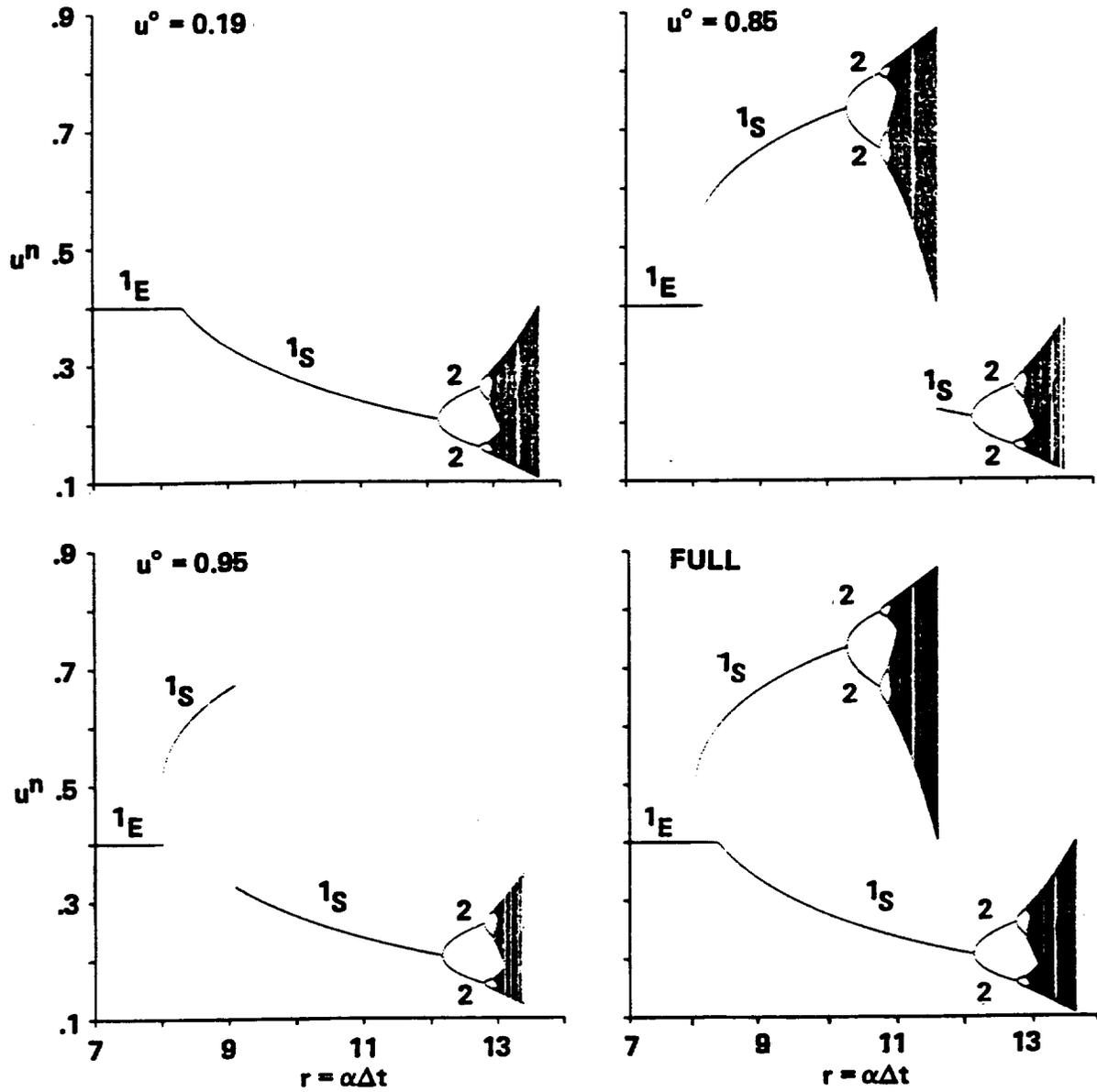


Figure 9. Bifurcation diagrams (transcritical) for Modified Euler (R-K 2) scheme applied to $u' = \alpha u(1-u)(0.4-u)$.

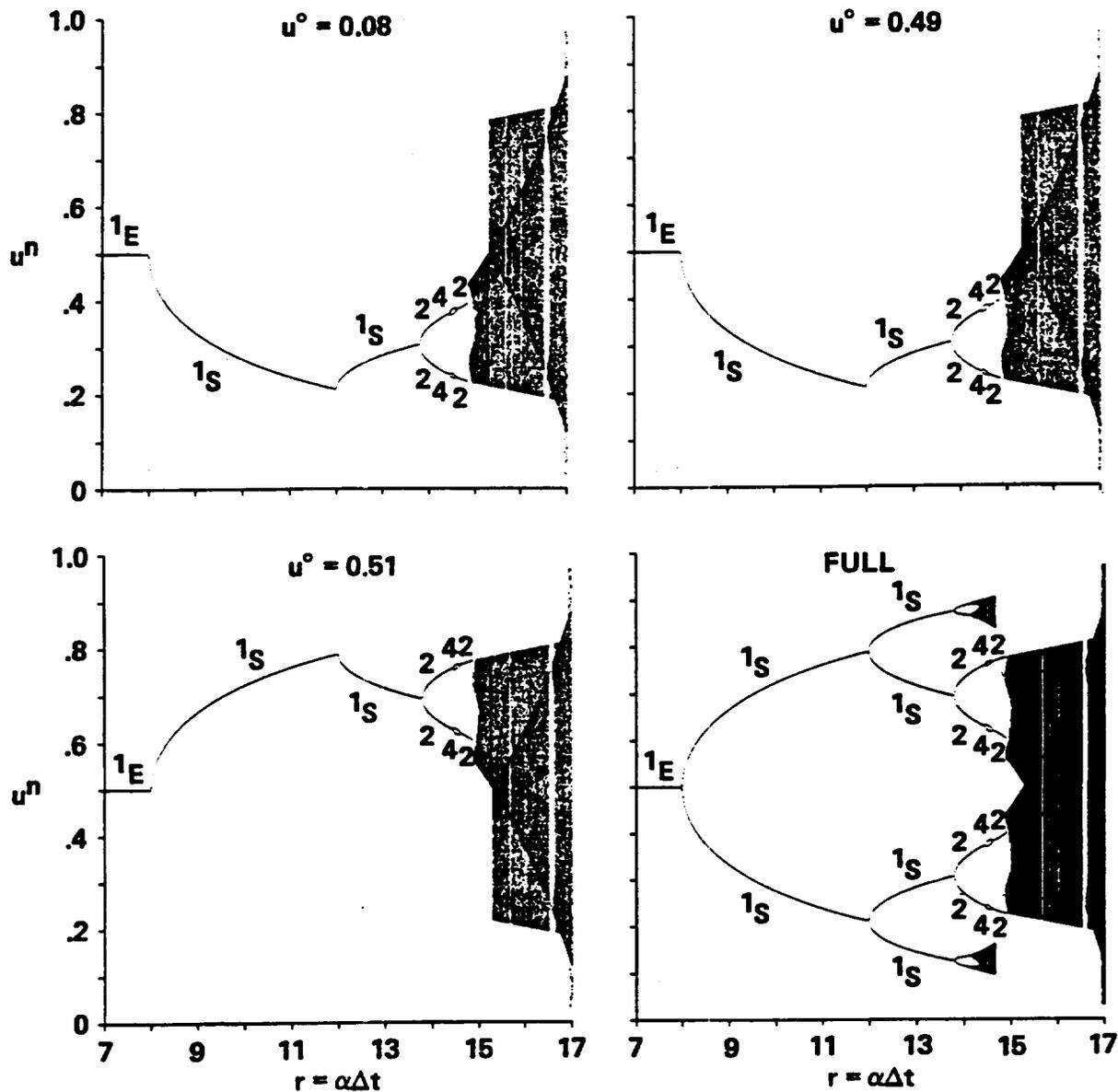


Figure 10. Bifurcation diagrams (supercritical) for Improved Euler (R-K 2) scheme applied to $u' = \alpha u(1 - u)(1/2 - u)$.

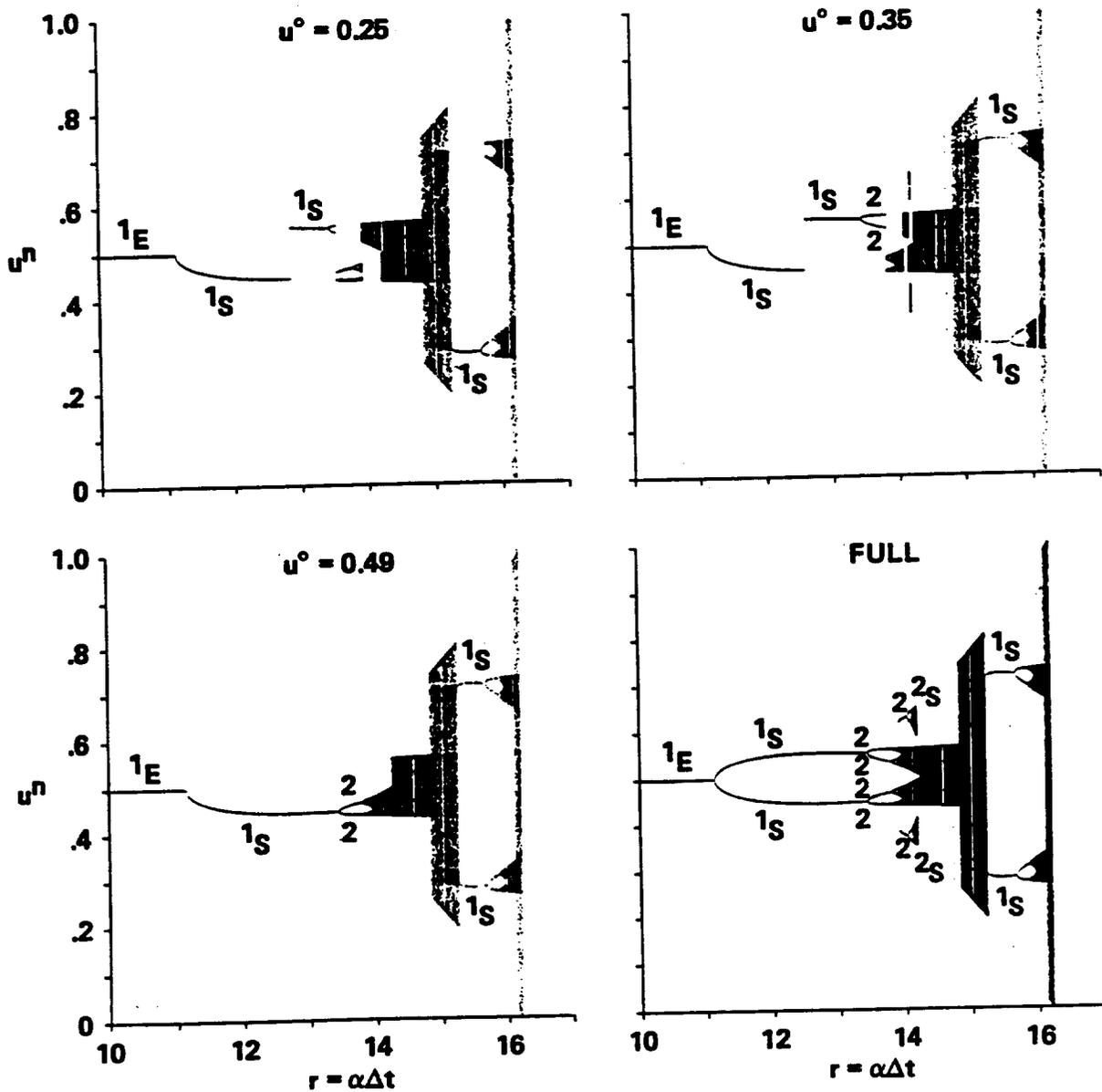


Figure 11. Bifurcation diagrams (supercritical) for Runge-Kutta 4th order scheme applied to $u' = \alpha u(1 - u)(1/2 - u)$.



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